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Pressure swing distillation of azeotropic mixture – A simulation study[☆]



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Received 22 January 2016; accepted 25 January 2016

Available online 6 February 2016

KEYWORDS

Pressure swing distillation;
Ethanol–Water mixture;
Simulation;
Azeotrope;
Aspen Plus

Summary The aim of this work is to simulate a pressure-swing distillation column for the separation and purification of ethanol from the ethanol–water binary system. The choice for this system is due to the importance of the ethanol–water separation. A steady-state equilibrium-stage model based on normalised MESH equations is used to simulate pressure-swing distillation column applied for the production of ethanol. All the work has been carried out using Aspen Plus simulator, version 13.2. Among the activity coefficient models available, the WILSON-RK model with binary parameters predicted by the Aspen Plus simulator is shown to be the most accurate to correlate the experimental vapor-/liquid equilibrium (VLE) data available for the ethanol–water system. The simulation has been satisfactorily carried out for a mixture of 20 mol% ethanol in water at 1 atm pressure and 90 °C with a molar flow rate of 100 kmol/h. The adjusting parameters include D/F ratio and reflux ratio of the two columns to get water purity of 99.5 mol% from the bottom of the Low Pressure Column (LPC) and the ethanol purity of 99.7 mol% from the bottom of High Pressure Column (HPC).

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Introduction

It has been observed that non-ideal mixtures of components forming an azeotrope are very difficult to separate to a purity beyond their azeotropic composition by using ordinary distillation. However separation of such non-ideal

mixtures is a very common process in chemical industries. In order to achieve high purity of the constituent components, enhanced techniques are employed which in turn render the distillation process highly expensive. Of the most common enhanced techniques like homogeneous azeotropic distillation (includes extractive distillation), heterogeneous azeotropic distillation, distillation using salt effects, or pressure-swing distillation (King, 1987) techniques, the simplest and most economical is the pressure swing distillation (PSD) technique which involves the use of two columns operating at different pressures (Winkle, 1967). A prerequisite for the PSD process is that the composition of azeotrope

[☆] This article belongs to the special issue on Engineering and Material Sciences.

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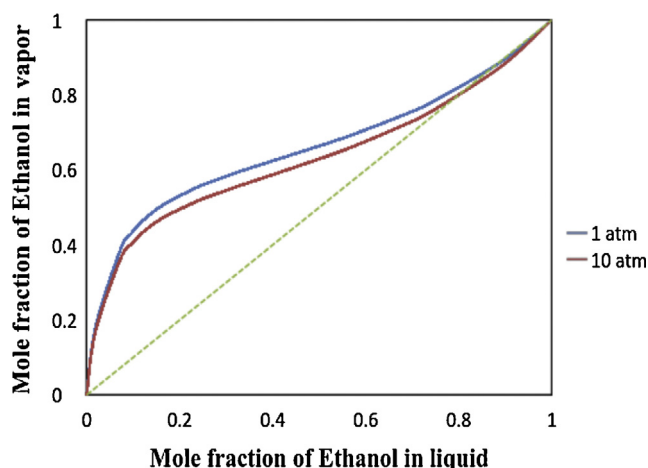


Figure 1 VLE data for ethanol water at different pressures.

should change significantly with the change in pressure. PSD is therefore, effective exclusively for those mixtures whose azeotropic compositions change with pressure so that feed components can be easily recovered (Mulia-Soto and Antonio, 2011; Luyben, 2012; Yamaki et al., 2012). Comparative studies show that the pressure swing distillation is a better option than extractive distillation from the standpoint of both economic considerations and product purity (Luyben, 2013; Wang et al., 2014).

In recent times, when the world is moving towards efficient unconventional and non-hazardous substitute for fuels, ethanol is emerging as a front runner. It finds its use in a plethora of other dimensions, such as its extensive use as a solvent and in the production of many chemicals and their intermediates. Its employability as a fuel has an abundant scope for growth. It is known that ethanol forms azeotrope with water and cannot be extracted to a high concentration from the aqueous solutions by ordinary distillation methods (Lei et al., 2002), therefore this mixture requires further processing in order to obtain high purity ethanol. Besides, the use of volatile organic compounds as solvents to separate the homogeneous binary azeotropic mixture of ethanol and water is hazardous to the environment. Hence the need for development of new, efficient and sustainable ways for the separation of ethanol–water azeotropic mixture arises. Pressure-swing distillation is one such technique for ethanol separation. It can be observed from Fig. 1 that the mixture of ethanol and water shows significant change from 0.885 to 0.812 in azeotropic composition on changing pressure, making it suitable for pressure swing distillation.

This study involves the progresses by first formulating the steady state mathematical model for pressure swing distillation process. The model equations are the steady state MESH equations. The model is then simulated using Aspen Plus 13.2 software. The design requirements are achieved by adjusting the parameters like D/F ratio and reflux ratio of the two columns, followed by the conclusions and recommendations for future work in the end.

Steady state simulation

In this simulation, both the columns consist of 30 stages (including a partial condenser with vapor distillate only

Table 1 RMSD values for different thermodynamic models using VLE data at 1 atm pressure.

Models	Parameters	WILSON	WILSON-RK	UNIFAC
RMSD values	y	0.0223	0.0194	0.0432
	T	0.0035	0.0033	0.2583

and a partial reboiler). Different thermodynamic models were analysed using Aspen Plus to predict the VLE data of ethanol–water system. The model that predicts the VLE data most accurately has been selected for the simulation.

Description of the problem

This work aims at obtaining high purity ethanol for a binary feed of ethanol and water by simulating the pressure swing distillation column. The problem specifications are as under:

- FEED: 100 kmol/h (20 mol% ethanol in water) at 90 °C and 1 atm, at stage no. 23 in LPC.
- LPC: operating pressure 1 atm; no. of stages = 30.
- HPC: operating pressure 10 atm; no. of stages = 30.

Vapor liquid equilibria

In order to use the simulation software, it is necessary to predict the VLE data accurately using the appropriate thermodynamic property model. Various thermodynamic property models like WILSON, WILSON-RK and UNIFAC have been tested to predict the VLE data of ethanol–water system at 1 atm. The predicted VLE data has been compared with the reported experimental VLE data (Perry and Green, 2001). The experimental data has been found to be in close proximity to that predicted by the WILSON-RK model and indicated by the RMSD values, calculated using Eq. (1), for vapor phase composition (y) and temperature (T) are given in Table 1.

$$\text{RMSD} = \sqrt{\frac{\sum (\text{relative error})^2}{\text{no. of data points}}} \quad (1)$$

Comparing the RMSD values in Table 1, it can be concluded that WILSON-RK model is most suitable to predict the VLE data of ethanol–water system correctly with a 1.94% error for vapor phase composition and 0.33% for phase temperature which is lowest among those obtained for WILSON and UNIFAC property models.

Simulation results

The LPC and HPC were simulated separately with a target distillate composition of 86.1 mol% ethanol (slightly less than the azeotropic composition at the column pressure) and 82.7 mol% ethanol (slightly more than the azeotropic composition at the column pressure) respectively and the bottom composition of 99.5 mol% water and 99.7 mol% ethanol respectively. The design specification tool under flow sheeting options of Aspen Plus has been used to meet the above

Table 2 Design specifications.

Target variable	Values	Adjustable variable	Values
Distillate composition from LPC	86.1 mol%	Reflux ratio in LPC	3.711
Distillate composition from HPC	82.7 mol%	Reflux ratio in HPC	4.29
Water purity from LPC	99.5 mol%	D/F ratio in LPC	0.55
Ethanol purity from HPC	99.7 mol%	D/F ratio in HPC	0.8

specifications. The adjustable variable to meet the above specifications are listed in [Table 2](#).

The next step of the PSD scheme, involved the combination of the two columns, with the distillate of LPC given as a feed to the HPC at feed stage no. 14 and the distillate of HPC recycled to the LPC at stage no. 13. The simulation was run with the same target and the adjustable variables as those for the simulation of the two columns separately. These targets were met with the reflux ratio of 3.711 in the LPC and 4.29 for the HPC and the D/F ratio of 0.55 in the LPC and 0.8 in the HPC.

Conclusions

The present work addresses the modelling and simulation of PSD scheme. As discussed above, the study is an effort to simulate a pressure swing distillation column for ethanol–water separation based on the model developed. The key objective of the proposed work is to simulate a pressure swing distillation process to obtain high purity ethanol. The ethanol water system has been chosen for the study because of its industrial importance. However, other systems may also be investigated in a similar manner. The LPC and HPC used in pressure swing distillation operate at 1 atm and 10 atm respectively. The simulation results indicate that the separation of ethanol–water azeotrope is feasible using PSD scheme, achieving high purity ethanol. The high purity ethanol (99.7 mol%) is obtained with the reflux ratio of 3.711 in the LPC and 4.29 for the HPC and the D/F ratio of 0.55 in the LPC and 0.8 in the HPC. As mentioned earlier, this

process is feasible in terms of environmental safety and economic viability. The work can be extended for reactive pressure swing distillation, pressure swing batch distillation, etc.

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